# Towards multi-state based computing using quantum-dot cellular automata


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**Abstract.** In this article we present an extended quantum-dot cellular automaton (QCA) cell. The extension is mainly focused on the enlargement of the range of possible states of a single QCA cell. In a QCA cell the electrons, owing to electrostatic repulsion, align along one of the two diagonal configurations that correspond to their maximal spatial separation. This gives the QCA cell the ability to encode two states or two logic values (0 and 1). By extending the QCA cell with four additional quantum dots we introduce the extended QCA (EQCA) cell and analyse its behaviour. Our approach is based on the semi-classical modelling approach. Using a special interpretation of electron configurations in the EQCA, the range of possible states is increased from two to three, which gives the EQCA cell the ability to encode the logic values (0, $\frac{1}{2}$ and 1). In our opinion the main benefit of this extension is the possibility for introducing "richer" processing and data storage capabilities without an increase in space requirements.


## 1 Introduction

With the seemingly endless miniaturisation of transistors and thus logic gates in integrated circuits the not so distant future reserves the challenge of integration in the nanometer scale. According to the well-known law, which originates from a prediction made by Gordon Moore forty years ago, the speed and complexity (i.e. the increase in the number of transistors per square inch) of integrated circuits doubles every 18 months. If this pace of miniaturisation increases or perhaps even if it does not subside, integration in the nanometer scale is to be expected in the next five to ten years [9]. The nanometer scale production of logic gates actually means that their assemblage will be on the scale of molecules and atoms. With this in mind it comes as no surprise that discussions about possible approaches to nanocomputing evoke terms as 'DNA computing', 'biomolecular computing', 'quantum computing', 'quantum-dot cellular automata', etc. In this article we focus on the latter.

The quantum-dot cellular automata (QCA) became interesting in the early 1990s, when Lent et al. [3] published the first results suggesting a possible interpretation of logic values 0 and 1 based on a configuration of a pair of tunnelled electrons contained in a QCA cell. The following research on the behaviour of spatial arrangements of QCA cells resulted in the implementation of the functionally complete set of logic functions [2] (i.e. the logic functions AND, OR and NOT) [10], as well as more complex structures and tools for their design [12]. The primary research focus was, in fact it still is, dedicated to the implementation of the classical two-valued logic and the corresponding computer structures associated with it. Indeed, the main building block (the QCA cell) is still capable of representing only 1 bit of data (i.e. either the logic value 0 or 1).

In this paper, we employ the semi-classical modelling approach [5] for the study of an eight-dot QCA or extended QCA (EQCA) cell. The semi-classical approach considers the electrons, which are contained in the cell, as classical particles that can arrange in the quantum dots in such a way as to minimize the total electrostatic energy of the system. The only added non-classical property is the ability of electrons to tunnel between adjacent dots. The model is developed with a numerical simulation that includes all possible configurations of electrons in each cell, with the only exception being the configurations in which more than one electron is confined in a single dot.

With the introduction of four additional quantum dots and a special interpretation of the corresponding electron configurations, we extend the (two-state) QCA towards a hypothetical three-state EQCA. With a possible realization in the nanoscale this approach would represent a giant leap forward in computer structures. Nevertheless, in our opinion, the main benefit is the shift towards novel research directions – from two-state to multi-state cells and the corresponding processing and data storage structures. With this the primary focus would be moved from the general miniaturisation towards the research on how to obtain "richer" processing and data storage capabilities without an increase in space requirements.

## 2 The semi-classical modelling approach

As already said, the semi-classical model for QCA cells is based on treating the electrons as classical particles, which can however tunnel between adjacent quantum dots [5]. The standard QCA cell has the structure presented in Fig. 1a[1] with four quantum dots separated by tunnelling barriers. Owing to electrostatic repulsion, the electrons will tend to align along one of the two distinct configurations, which correspond to their maximum spatial separation. In the absence of external electric fields, these configurations will have exactly the same energy, while in the presence, for example, of a nearby cell with a well-defined charge distribution, one of them will be energetically favoured. Apart from these two there are also four more possible configurations; due to the very large associated electrostatic energy the configurations in which more than one electron is confined in a single dot are not considered. This means that there is a total of six

[1] For reasons of simplicity all diagrams, except Figs. 1a and 4a, display only the electron configurations and display neither the quantum dots nor the tunnelling barriers.

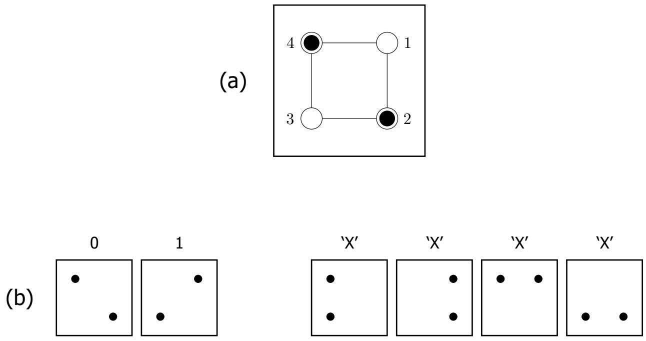



**Fig. 1.** Layout of a four-dot QCA cell with two electrons (a) and the corresponding possible configurations for two electrons in a cell (b).

configurations, as presented in Fig. 1b. Traditionally the two diagonal configurations are associated with logic values 0 and 1 (the configuration with electrons in dots 2 and 4 with 0 and the one with electrons in dot 1 and 3 with 1). The rest of all possible configurations are not associated with any logic value; they are marked as 'X' states.

In all of our simulations a positive background charge (in the case of an $m$-dot QCA, containing two electrons, the charge $\frac{2e}{m}$, where $e$ is the electron charge), is assumed in each dot, in order to keep the cell overall neutral. This is necessary to avoid undesired effects associated with the monopole electric field component that would be produced by a non-neutral cell. The latter would as a result tend to push all electrons contained in the nearby cell towards the further side of the cell (i.e. toward the right side of it if the nearby cell is on the right). This means that the total electrostatic energy of an array of cells is, in the semi-classical model, expressed as the energy of a system of point charges

$$E = \sum_{i \neq j} \frac{\rho_i \rho_j}{4\pi\varepsilon_0\varepsilon_r r_{ij}}, \tag{1}$$

where $\rho_i$ is the charge associated with the $i$th dot, $r_{ij}$ is the distance between dot $i$ and dot $j$, $\varepsilon_0$ is the vacuum permittivity, and $\varepsilon_r$ is the relative permittivity of the medium (we consider the case of GaAs/AlGaAs, assuming a uniform relative permittivity of 12.9). Repeating the evaluation of the total energy for all possible configurations, the ground state and the distribution of energy values can be determined. In the case of an arrangement of $n$ $m$-dot cells, each containing two electrons, this means an exhaustive exploration of $\binom{m}{2}^n$ possible configurations.

## 3 QCA structures and QCA based switching

A *QCA structure* is a spatial arrangement of QCA cells performing a dedicated function. It can be decomposed into three segments. The first segment represents the input cells or *drivers*. In a physical sense these are usually located at the edge of the structure; their states are enforced by means of external electric field sources. The second segment is represented by the *internal* cells. With respect to their physical arrangement within the structure they transmit data from the input cells towards the third segment, the output or *target* cells. Typically the data that is input into the QCA structure is transformed with respect to the spatial arrangement of the internal cells. A more detailed description of the temporal dynamics and synchronisation mechanisms can be found in [3, 4, 6, 11]. As no direct connections can be made to internal cells and data can enter or leave the structure only on its edges, this scheme corresponds to edge-driven computation. In other words: the above means that the problem of designing a desired input/output transformation translates into the problem of finding the correct spatial arrangement of cells.

If several cells are lined up to form a wire, and a given logic value is enforced for the first cell, it will propagate along the wire in a domino fashion [10], until all cells have reached the same configuration, as presented in Fig. 2. As this

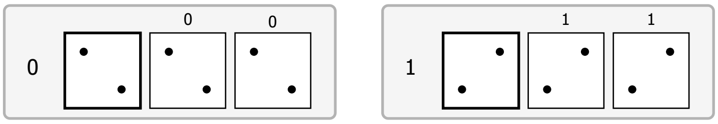



**Fig. 2.** The binary wire. Propagation of electron charge distribution along a line of QCA cells.

means that, effectively, the logic value 0 or 1 enforced (input) on one end of the wire is propagated to the other end of it (output), the wire is called a binary wire.

Nevertheless, the basics of designing QCA structures originate from the desire to find arrangements of QCA cells that implement the basic logic functions AND, OR and NOT [2]. This first succeeded to Lent et al. [3]. A QCA inverter, or NOT, is obtained by offsetting the target cell from the driver cell by 45deg as presented in Fig. 3. In this case a given logic value enforced to the driver will be inverted in the target cell, the logic value 0 thus producing 1 and vice versa.

The AND and OR function, on the other hand, are constructed as an intersection of three binary wires [8]. This produces the topology presented in Fig. 3 denoted as the QCA *majority gate*. In this gate the three inputs (S, X and Y) 'vote' on the configuration of the internal cell (T), and the majority wins. The configuration of the internal cell is then propagated toward the output cell (M). One of the inputs (in our case S) can be used as a programming input to select the AND or OR function. If the programming input is the logic value 0, then the gate behaves as the AND logic function, whereas if it is the logic value 1, then the gate behaves as the OR logic function.

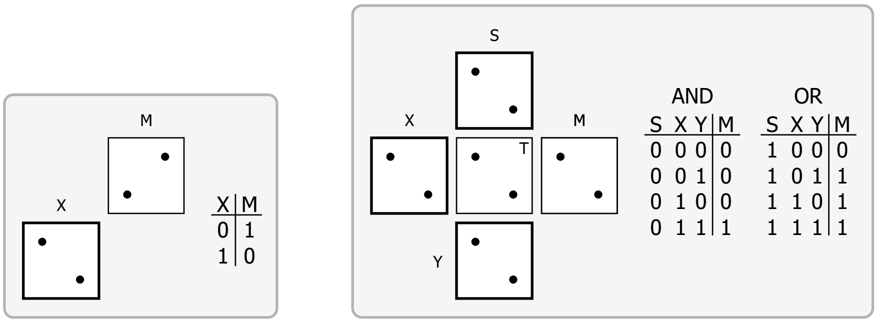



**Fig. 3.** The QCA inverter (left) and the QCA majority gate (right).

The ability to transfer data and the functionally complete set of logic functions gives us the ability to construct any given switching structure and thus enables QCA computation.

## 4 Towards a multi-state QCA cell

### 4.1 The EQCA cell

The EQCA cell is an eight-dot QCA cell with the structure presented in Fig.4a. The dots are evenly distributed in a circular fashion, and again separated by tunnelling barriers. As in the QCA cell the electrons will, due to the electrostatic repulsion, tend to align along one of the distinct configurations that correspond to their maximal spatial separation. In the absence of external electric fields, these configurations will have exactly the same energy[2], while in the presence, for example, of a nearby cell with a well-defined charge distribution, one of them will be again energetically favoured. There are 4 distinct configurations with maximal spatial separation between electrons. Additionally there are also 24 more possible configurations. Again, the configurations in which more than one electron is confined in a single dot are not considered, due to the very large associated electrostatic energy. This means that there is a total of 28 configurations, as presented in Fig. 4b. We shall denote the diagonal configurations as configuration 'A' (i.e. electrons in dots 2 and 4) and configuration 'B' (i.e. electrons in dots 1 and 3). The vertical configuration (i.e. electrons in dots 5 and 7) and the horizontal configuration (i.e. electrons in dots 6 and 8) will, on the other hand, be denoted as configurations 'C' and 'D' respectively. The rest of all possible configurations will be marked as 'X' states.

[2] Have in mind that our primary interest is extending the functionality of a cell for expanding its processing capabilities. This means that currently both the process of physical construction and the process of forcing/detecting a charge distribution are taken out of account.

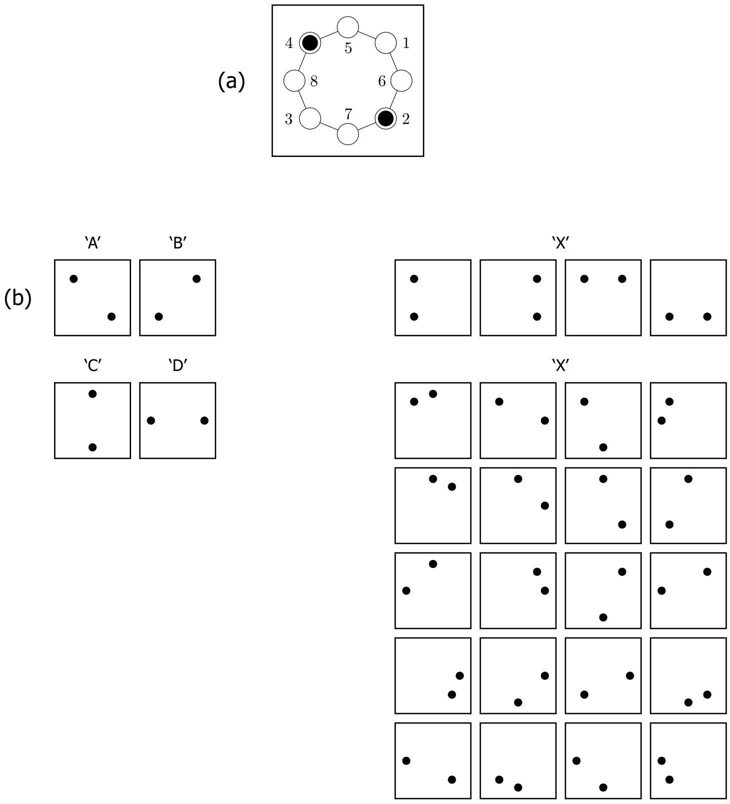



**Fig. 4.** Layout of an eight-dot EQCA cell with two electrons (a) and the corresponding possible configurations for two electrons in a cell (b).

If several cells are lined up to form a wire and either configuration 'A' or 'B' is enforced for the first cell, it will propagate along the wire, until all cells have reached the same configuration. Nevertheless if the enforced configuration is either 'C' or 'D' it will propagate along the wire in an alternating fashion, such as for example CDCDCDC... (see Fig. 5). This means that if we associate configuration 'A' with the logic value 0 and configuration 'B' with the logic value 1, in fact by retaining the associations of the classical QCA cell we retain also the binary wire capability. Additionally, if we interpret both configurations 'C' and 'D' as the logic value $\frac{1}{2}$ we end up with a three-state wire; we can effectively propagate the logic values 0, $\frac{1}{2}$ and 1. This ability opens up a whole new spectrum of possible processing capabilities. We are no longer talking about a binary universe, binary logic and binary processing but we are stepping into a three-state universe towards three-valued logic, and three-valued processing.

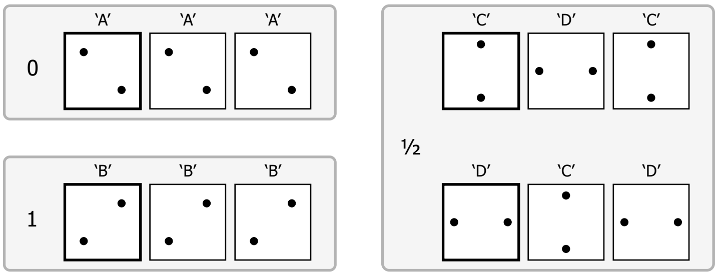



**Fig. 5.** The three-state wire. Propagation of electron charge distribution along a line of EQCA cells.

### 4.2 EQCA based switching

Multi-valued logic is a term used to describe all logics of three or more values. Three-valued logic, as a contrast to two-valued logic, which allows only logic values 0 (false) and 1 (true), allows also for the third option $\frac{1}{2}$ (possible). The truth tables for three-valued logic functions were set up by the Polish mathematician Jan Łukasiewicz [1] in the 1920s as a generalization of the corresponding truth tables found in two-valued logic (see Fig. 6). In multi-valued logic, however, the

NOT

| X | M |
|---|---|
| 0 | 1 |
| ½ | ½ |
| 1 | 0 |

AND

| X | Y | M |
|---|---|---|
| 0 | 0 | 0 |
| 0 | ½ | 0 |
| 0 | 1 | 0 |
| ½ | 0 | 0 |
| ½ | ½ | ½ |
| ½ | 1 | ½ |
| 1 | 0 | 0 |
| 1 | ½ | ½ |
| 1 | 1 | 1 |

OR

| X | Y | M |
|---|---|---|
| 0 | 0 | 0 |
| 0 | ½ | ½ |
| 0 | 1 | 1 |
| ½ | 0 | ½ |
| ½ | ½ | ½ |
| ½ | 1 | 1 |
| 1 | 0 | 1 |
| 1 | ½ | 1 |
| 1 | 1 | 1 |

**Fig. 6.** Łukasiewicz truth tables for tree-valued logic functions NOT, AND and OR.

logic functions NOT, AND and OR are typically expressed as

$$\mathrm{NOT}(x) = 1 - x, \quad \mathrm{AND}(x, y) = \min(x, y), \quad \mathrm{OR}(x, y) = \max(x, y). \quad (2)$$

Needless to say, these equations hold also for Łukasiewicz's three-valued logic. The above means that the problem of processing with EQCA cells translates into searching for EQCA structures that implement these equations.

Our approach to this problem was the most obvious one. To test if the QCA structures, which are used to implement the two-valued logic functions would give the correct results even when constructed using EQCA cells.

Surprisingly enough, the inverter, or NOT, worked perfectly, as shown in Fig. 8, giving the correct output for any given input. In the case of input configuration ‘A’ the output configuration was ‘B’ and vice versa. Then again, if the enforced input configuration was either ‘C’ or ‘D’, the output configuration did not change.

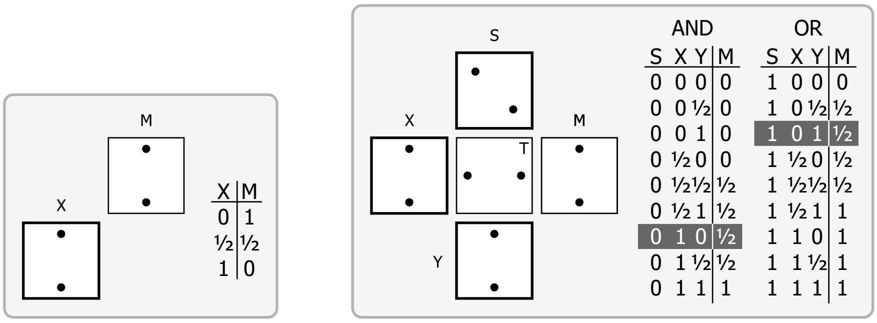
The EQCA majority gate, on the other hand, proved to be a bit more troublesome. Indeed in the EQCA case the full range of possible input configurations increases from $2^3 = 8$, in the QCA case, to $4^3 = 64$.[3] From Fig. 7 it becomes

| | S | X | Y | T | M | | S | X | Y | T | M | S | X | Y | T | M | S | X | Y | T | M |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AND(0,0) | A | A | A | A | A | OR(0,0) | B | A | A | A | A | C | A | A | A | A | D | A | A | C | D |
| AND(0,1) | A | A | B | A | A | OR(0,1) | B | A | B | C | D | C | A | B | D | C | D | A | B | C | D |
| AND(0,½) | A | A | C | A | A | OR(0,½) | B | A | C | D | C | C | A | C | D | C | D | A | C | A | A |
| | A | A | D | C | D | | B | A | D | C | D | C | A | D | A | A | D | A | D | C | D |
| AND(1,0) | A | B | A | C | D | OR(1,0) | B | B | A | B | B | C | B | A | D | C | D | B | A | C | D |
| AND(1,1) | A | B | B | B | B | OR(1,1) | B | B | B | B | B | C | B | B | B | B | D | B | B | C | D |
| AND(1,½) | A | B | C | D | C | OR(1,½) | B | B | C | B | B | C | B | C | D | C | D | B | C | B | B |
| | A | B | D | C | D | | B | B | D | C | D | C | B | D | B | B | D | B | D | C | D |
| AND(½,0) | A | C | A | A | A | OR(½,0) | B | C | A | D | C | C | C | A | D | C | D | C | A | C | D |
| AND(½,1) | A | C | B | D | C | OR(½,1) | B | C | B | B | B | C | C | B | D | C | D | C | B | C | D |
| AND(½,½) | A | C | C | D | C | OR(½,½) | B | C | C | D | C | C | C | C | D | C | D | C | C | D | C |
| | A | C | D | C | D | | B | C | D | C | D | C | C | D | D | C | D | C | D | C | D |
| | A | D | A | C | D | | B | D | A | C | D | C | D | A | A | A | D | D | A | C | D |
| | A | D | B | C | D | | B | D | B | C | D | C | D | B | B | B | D | D | B | C | D |
| | A | D | C | A | A | | B | D | C | B | B | C | D | C | D | C | D | D | C | C | D |
| | A | D | D | C | D | | B | D | D | C | D | C | D | D | C | D | D | D | D | C | D |

**Fig. 7.** The full range of possible input configurations for the EQCA majority gate.

evident that, when using the full range of all possible input configurations, the majority gate does not work as intended. However, if we suppose that configuration ‘D’ (see Fig. 4b) is merely a processing configuration (i.e. if we assume that it is not allowed for input cells, but is allowed only for internal cells) then we obtain the truth table presented in Fig. 8. This precondition is easily met. Indeed, if care is taken that, whenever a logic value is required to be transmitted over a EQCA wire, the wire is constructed from an odd number of EQCA cells, then the output cell will always assume the same configuration as the input cell, even in the case when the input configuration is ‘C’ or ‘D’. The obtained truth table is remarkably similar to the one set up by Łukasiewicz (compare Figs. 6 and 8). The only two problematic input combinations are $\mathrm{AND}(1,0)$ and $\mathrm{OR}(0,1)$ which both return $\frac{1}{2}$ instead of returning 0 and 1 respectively. Nevertheless, in both cases the output cell reaches configuration ‘D’, as shown in Fig. 9. Since configuration ‘D’ is reached only from these two input combinations, a possible solution for obtaining the required truth table would be a special additional EQCA structure. Its sole objective would be to translate configuration ‘D’ into the correct output value and it would be employed only in the case when the output configuration is ‘D’. Our current research is focused upon obtaining such a structure.

[3] With the given interpretation of configurations ‘C’ and ‘D’ (i.e. both as the logic value $\frac{1}{2}$), the number of distinct input combinations is in fact $3^3 = 27$.




| X | M |
|---|---|
| 0 | 1 |
| ½ | ½ |
| 1 | 0 |

AND

| S | X | Y | M |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | ½ | 0 |
| 0 | 0 | 1 | 0 |
| 0 | ½ | 0 | 0 |
| 0 | ½ | ½ | ½ |
| 0 | ½ | 1 | ½ |
| 0 | 1 | 0 | ½ |
| 0 | 1 | ½ | ½ |
| 0 | 1 | 1 | 1 |

OR

| S | X | Y | M |
|---|---|---|---|
| 1 | 0 | 0 | 0 |
| 1 | 0 | ½ | ½ |
| 1 | 0 | 1 | ½ |
| 1 | ½ | 0 | ½ |
| 1 | ½ | ½ | ½ |
| 1 | ½ | 1 | 1 |
| 1 | 1 | 0 | 1 |
| 1 | 1 | ½ | 1 |
| 1 | 1 | 1 | 1 |

**Fig. 8.** The EQCA inverter (left) and the EQCA majority gate (right).

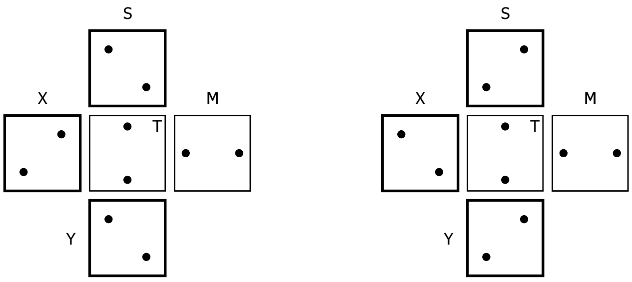



**Fig. 9.** The two erroneous input/output configurations for the EQCA majority gate when used for implementing the three-valued AND (left) and OR (right) logic functions.

## 5 Conclusion

In this article we present an extended quantum dot cellular automaton cell. The extension focuses on the enlargement of the range of possible states of a single cell. More specifically we present an eight-dot QCA, which together with a specific interpretation of electron configurations defines a three-state EQCA cell that is capable of transmitting logic values 0, $\frac{1}{2}$ and 1 over a three-state wire. Additionally we highlight the faced challenges and present some of the possible solutions for its application to the design of future processing structures based on multi-valued logic. The primary goal of this research is in the promotion of the idea to switch the focus from pure miniaturisation towards research for a better use of the existing level of miniaturisation. The era of analytical top-down approaches is nearing its end and we are entering the era of bottom-up synthesis approaches. Indeed it would be unsound to assume that in the years to come both the ethical as well as the technical aspects of miniaturisation will keep on flourishing with the same pace [7].

## References


1. Borkowski L. (ed.): Jan Lukasiewicz: Selected Works. North-Holland Publishing Company, Amsterdam (1970)
2. Kohavi Z.: Switching and finite automata theory. McGraw-Hill Inc., New York (1978)
3. Lent C.S., Tougaw P.D., Porod W., Bernstein G.H.: Quantum cellular automata. Nanotechnology **4** (1993) 49–57
4. Lent C.S., Tougaw P.D.: Lines of interacting quantum-dot cells: A binary wire. J. Appl. Phys **74** (1993) 6227–6233
5. Macucci M., Iannaccone G., Francaviglia S., Pellegrini B.: Semiclassical simulation of quantum cellular automaton cells. Int. J. Circ. Theor. Appl. **29** (2001) 37–47
6. Niemier M.T., Kogge P.M.: Origins and motivations for design rules in QCA, in: Nano, Quantum and Molecular Computing, Ed. S.K. Shukla and R.I. Bahar, Kluwer Academic Publish. (2004) 267–293
7. Phoenix C., Drexler E.: Safe exponential manufacturing. Nanotechnology **15** (2004) 869–872
8. Snider G.L, Orlov A.O., Amlani I., Bernstein G.H.: Quantum-dot cellular automata: Line and majority logic gate. Jpn. J. Appl. Phys **38** (1999) 7227–7229
9. Steane S., Rieffel E.: Beyond bits: The future of quantum information processing. IEEE Computer **1** (2000) 38–45
10. Tougaw P.D., Lent C.S.: Logical Devices Implemented Using Quantum Cellular Automata. J. Appl. Phys. **75** (1994) 1818–1825
11. Tougaw P.D., Lent C.S.: Dynamic behaviour of quantum cellular automata. J. Appl. Phys. **80** (1996) 4722–4736
12. Walus K., Dysart T.J., Jullien G.A., Budiman R.A.: QCADesigner: A rapid design and simulation tool for quantum dots cellular automata. IEEE Transactions on Nanotechnology **3** (2004) 26–31